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Guide

Guide for the Verification and Validation of Computational Fluid Dynamics Simulations

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Abstract

This document presents guidelines for assessing the credibility of modeling and simulation in computational fluid dynamics. The two main principles that are necessary for assessing credibility are verification and validation. Verification is the process of determining if a computational simulation accurately represents the conceptual model, but no claim is made of the relationship of the simulation to the real world. Validation is the process of determining if a computational simulation represents the real world. This document defines a number of key terms, discusses fundamental concepts, and specifies general procedures for conducting verification and validation of computational fluid dynamics simulations. The document's goal is to provide a foundation for the major issues and concepts in verification and validation. However, this document does not recommend standards in these areas because a number of important issues are not yet resolved. It is hoped that the guidelines will aid in the research, devced in any form, in an electronic retrieval system or otherwise, without prior written permissielopment and use of computational fluid dynamics simulations by establishing common terminology and methodology for verification and validation. The terminology and methodology should also be useful in other engineering and science disciplines.

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FOREWORD

The American Institute of Aeronautics and Astronautics (AIAA) Standards Program sponsored development of this document, *Guide for the Verification and Validation of Computational Fluid Dynamics Simulations*. This document originated within the AIAA Computational Fluid Dynamics Committee on Standards, which is composed of AIAA members and others who are not affiliated with AIAA. Committee members come from industry, government, and academia, and serve voluntarily without compensation. This document represents a consensus of the Committee's opinions on the terminology and methodology for verification and validation of computational fluid dynamics (CFD) simulations.

This document is primarily a synthesis of opinions from the published literature on verification and validation in modeling and simulation. Perspectives from a wide variety of sources were assembled in order to develop the most useful, self-consistent, and logical framework. Even though there is a variety of opinion on verification and validation in the literature, there is increasing agreement on the fundamental aspects. It is hoped that this document will promote consensus on the major issues among the CFD community at large.

The goal of this document is to support researchers, developers, and users of CFD by establishing common terminology and methodology for verification and validation of CFD simulations. The terminology and methodology should also be useful in other engineering and science disciplines.

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This document is subject to change based on developments in the state-of-the-art and on comments received from readers. Comments are welcome from any interested party, regardless of membership affiliation with AIAA. Comments should be directed to

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The first draft of this document was prepared by Unmeel B. Mehta. This draft was prepared by William L. Oberkampf, Munir M. Sindir, and A. Terrence Conlisk. A number of comments and suggestions for improvements of this document were made by members of the AIAA Computational Fluid Dynamics Committee on Standards and by several interested individuals who were not on the Committee. We appreciate and value all input provided.

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EXECUTIVE SUMMARY

Computer simulations of fluid flow processes are now used to design, investigate, and operate engineered systems and to determine the performance of these systems under various conditions. Computational fluid dynamics (CFD) simulations are also used to improve understanding of fluid physics and chemistry, such as turbulence and combustion, and to aid in weather prediction and oceanography. Although CFD simulations are widely conducted in industry, government, and academia, there is presently little agreement on procedures for assessing their credibility. These guidelines are predicated upon the notion that there is no fixed level of credibility or accuracy that is applicable to all CFD simulations. The accuracy level required of simulations depends on the purposes for which the simulations are to be used.

The two main principles that are necessary for establishing credibility are verification and validation. As defined here, verification is the process of determining that a model implementation accurately represents the developer's conceptual description of the model and the solution to the model. Validation is defined as the process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model. These definitions point out that verification and validation (V&V) are ongoing activities that do not have a clearly defined completion point. Completion or sufficiency is usually determined by practical issues such as budgetary constraints and intended uses of the model. All encompassing proofs of correctness, such as those developed in mathematical analysis, do not exist in complex modeling and computational simulation. The definitions of V&V also stress the evaluation of accuracy. In verification activities, accuracy is generally measured with respect to benchmark solutions of simplified model problems. In validation activities, accuracy is measured with respect to experimental data, i.e., reality.

Uncertainty and error can be considered as the broad categories that are normally associated with loss in accuracy in modeling and simulation. Uncertainty is defined as a potential deficiency in any phase or activity of the modeling process that is due to lack of knowledge. Lack of knowledge is commonly caused by incomplete knowledge of a physical characteristic or parameter, as in the inadequate characterization of the distribution of surface roughness on a turbine blade. Lack of knowledge can also be caused by the complexity of a physical process, for example, turbulent combustion. Error is defined as a recognizable deficiency in any phase or activity of modeling and simulation that is not due to lack of knowledge. Error can be categorized as either acknowledged or unacknowledged. Examples of acknowledged errors are round-off error in a digital computer and physical approximations made to simplify the modeling of a physical process. Unacknowledged errors are blunders, or mistakes, such as programming errors.

In the context of verification and validation, the meaning of the word “prediction” is restricted from its general usage to consider the history of validation activities with the CFD model. Prediction is defined as the use of a CFD model to foretell the state of a physical system under conditions which the CFD model has not been validated. This definition of prediction is a subset of the general meaning of prediction because it eliminates past comparisons with experimental data. If this restriction is not made, then there is little value in saying that one has reproduced agreement with experimental data. The processes or activities of V&V should be viewed as historical statements, i.e., reproducible evidence that a model has achieved a given level of accuracy in the solution of specified problems. Viewed in this light, it becomes clear that the V&V processes do not directly make claims about the accuracy of predictions.

The fundamental strategy of verification is the identification and quantification of error in the computational solution. In CFD simulations, there are four predominant sources of error, namely insufficient spatial discretization convergence, insufficient temporal discretization convergence, lack of iterative convergence, and computer programming. The most important activity in verification testing is systematically refining the grid size and time step. The objective of this activity is to estimate the discretization error of the numerical solution. As the grid size and time step approach zero, the discretization error should monotonically approach zero. When the monotonic region has been demonstrated, Richardson's extrapolation can be used to estimate zero-grid spacing and time step. In most cases, CFD equations are highly nonlinear, and the vast majority of methods of solving these equations requires iteration. These iterations normally occur in two situations: 1) globally, i.e, over the entire domain, for boundary value problems; and 2) within each time step for initial-boundary value problems. In verification testing, the sensitivity of the solution to the magnitude of the convergence criteria should be varied, and a value should be established that is consistent with the objectives of the simulation. In verification activities, comparing a computational solution to a highly accurate solution is the most accurate and reliable way to quantitatively measure the error in the computational solution. However, highly accurate solutions are known only for a relatively small number of simplified problems. These highly accurate solutions can be classified into three types: analytical solutions, benchmark numerical solutions to ordinary differential equations, and benchmark numerical solutions to partial differential equations. As one moves from analytical solutions to ODE solutions to PDE solutions, the accuracy of the benchmark solutions clearly becomes more of an issue.

The fundamental strategy of validation is the identification and quantification of error and uncertainty in the conceptual and computational models. The recommended validation method is to employ a building-block approach. This approach divides the complex engineering system of interest into three progressively simpler phases: subsystem cases, benchmark cases, and unit problems. The strategy in this approach is the assessment of how accurately the computational results compare with experimental data (with quantified uncertainty estimates) at multiple levels of complexity. Each phase of the process represents a different level of flow physics coupling and geometrical complexity. The complete system consists of the actual hardware or system for which a validated CFD tool is needed. Thus all the geometric and flow physics effects occur simultaneously; commonly, the complete system includes multidisciplinary physical phenomena. Subsystem cases represent the first decomposition of the actual hardware into simplified or partial flow paths. Each of these cases commonly exhibits restricted geometric or flow features compared to the complete system. Benchmark cases represent another level of successive decomposition of the complete system. For these cases, separate hardware is fabricated to represent key features of each subsystem. The benchmark cases are geometrically simpler than those at the subsystem level, as only two separate features of the flow physics and two flow features are commonly coupled in the benchmark cases. Unit problems represent the total decomposition of the complete system. High-precision, special-purpose hardware is fabricated and inspected. Unit problems are characterized by very simple geometries, one flow-physics feature, and one dominant flow feature.

1. INTRODUCTION

1.1 Background

Computational fluid dynamics (CFD) is an emerging technology. It is the merger of the classical branches of theoretical and experimental science, with the infusion of the modern element of numerical computation. The progress in CFD during the last 40 years has been extraordinary. Much of this progress has been driven by the phenomenal increases in digital computing speed. The cost of computation has decreased roughly five orders of magnitude since 1955 [1]. The power of digital computing has transformed research and engineering in fluid mechanics, just as it has in virtually all fields of human endeavor.

Computer simulations of fluid flow processes are now used to design, investigate, and operate engineered systems and to determine their performance under various conditions. The systems of interest can be existing or proposed systems operating at design conditions, off-design conditions, failure-mode conditions, or accident scenarios. CFD simulations are also used to improve understanding of fluid physics and chemistry, such as turbulence and combustion, and to aid in weather prediction and oceanography. In addition, these types of simulations are employed as an aid in developing public policy, in preparing safety procedures, and in determining legal liability. Researchers, developers, and users of CFD simulations, as well as those affected by decisions based on these simulations, are all justly concerned with the credibility of the results.

Although CFD simulations are widely conducted in industry, government, and academia, there is presently little agreement on procedures for assessing their credibility. The two main principles that are necessary for assessing credibility are verification and validation. As defined here, verification is the process of determining if a computational simulation accurately represents the conceptual model; but no claim is made of the relationship of the simulation to the real world. Validation is the process of determining if a computational simulation represents the real world. Verification determines whether the problem has been solved correctly, whereas validation determines whether the correct problem has been solved. A consistent and logical framework for verification and validation is needed to derive the greatest benefit from CFD modeling and simulation.

1.2 Scope

The fundamental strategy of verification and validation is the assessment of error and uncertainty in the computational simulation. The required methodology is a complex process because it must assess errors and uncertainties originating in all three roots of CFD: theory, experiment, and computation. Given these diverse perspectives, it is common to find disagreement and conflict in the terminology of verification and validation. Furthermore, because fluid dynamics is dominated by nonlinear phenomena; it is common for multiple nonlinearities to be strongly coupled. This introduces significant difficulties in modeling the phenomena and in solving the resulting nonlinear partial differential equations.

This document builds primarily on terminology established by the Society for Computer Simulation and the Defense Modeling and Simulation Office of the Department of Defense [2-4]. Concerning the methodology of verification and validation, however, there are no publications that present general and comprehensive procedures in the computational sciences. It is fair to call the present state-of-the-art for verification and validation methodology *ad hoc*. The purpose of this document is to promote the establishment of basic terminology and methodology for the verification and validation of CFD simulations.

It is important to emphasize that this document presents guidelines for verification and validation of CFD simulations, not standards. The AIAA Computational Fluid Dynamics Committee on Standards unanimously believes that the state-of-the-art in CFD has not developed to the point where standards can be written. The Committee is dedicated to revising this document on a regular basis, following the same approach taken in the preparation of this document. That is, revisions will be made with broad input from other AIAA Technical Committees and any individuals interested in the advancement of CFD.

A few archival journals have developed editorial policies pertaining to the control of numerical accuracy in fluid flow simulations [5-8]. Numerical accuracy is one aspect of verification and validation, but there are many more aspects as discussed in these guidelines. While it is desired that these guidelines can lead to enhancing the quality of work published in journals, publication-related issues are not specifically within the scope of this document. It should also be made clear that the procedures described in these guidelines are not meant to be necessary conditions for publication of manuscripts in any of the AIAA journals or at any conferences sponsored by AIAA.

These guidelines are predicated upon the notion that there is no fixed level of credibility or accuracy that is applicable to all CFD simulations. The accuracy level required of simulations depends on the purposes for which the simulations are to be used. In effect, all simulations do not need to demonstrate high accuracy. For example, absolute or high accuracy simulations are not normally required for engineering activities; such simulations only need to be useful, not perfect. The required level of accuracy must be determined for each use of the simulation. Typical practicalities affecting the accuracy obtained are cost, schedule, and safety implications of the simulation.

1.3 Outline

Section 2 defines a number of fundamental terms, such as model, error, uncertainty, and prediction. The reasoning for choosing the definitions and the implications of the definitions are also discussed. Section 3 describes the methodology for verification, which is applicable to discretized solutions of the partial differential equations of fluid dynamics. The recommended procedures apply to finite difference methods, finite element methods, finite volume methods, spectral methods, and boundary element methods. The uses of analytical solutions and benchmark numerical solutions in verification are presented, along with issues related to spatial and time-step convergence and to iterative convergence. Section 4 discusses the methodology for validation. The validation of CFD simulations is recognized by many as consisting of a hierarchy of comparisons with experimental data. In this methodology, the hierarchical elements of validation are unit problems, benchmark cases, subsystem cases, and the complete system. Emphasizing a practical approach for complex engineering systems, the validation methodology also points out similarities and distinctions between validation and calibration and discusses requirements for the design and execution of validation experiments.

2. CONCEPTS AND TERMINOLOGY

There has been a long history of efforts to establish the basic concepts and terminology in modeling and computational simulation. The identification of the fundamental issues and debates began decades ago in the operations research (OR) community—long before there was such concern in the CFD community [2, 9-14]. In the preparation of this guide, definitions and concepts developed by a number of organizations were studied: the Department of Defense (DoD) [3, 4], the Institute of Electrical and Electronics Engineers [15, 16], the American Nuclear Society [17], and the International Standards Organization [18, 19]. The following subsections define and discuss a set of key terms for modeling and simulation in CFD.

2.1 Modeling and Simulation

The terms *model*, *modeling*, and *simulation* are used in a wide range of disciplines. Consequently, these terms have a wide range of meanings that are both context-specific and discipline-specific [16, 20]. As used in this guide, the terms are defined as follows:

> *Model*: A representation of a physical system or process intended to enhance our ability to understand, predict, or control its behavior.
>
> *Modeling*: The process of construction or modification of a model.
>
> *Simulation*: The exercise or use of a model. (That is, a model is used in a simulation.)

The basic phases of modeling and simulation have been identified by the OR community. Figure 1 shows these basic phases and processes as adopted by the Society for Computer Simulation (SCS) [2]. Note that all the definitions of terms provided in this document are consistent with the SCS framework shown in Fig. 1. The present guidelines go beyond Fig. 1 in a number of respects, but our extensions are consistent with the general view of the SCS.

Figure 1 identifies two types of models: a conceptual model and a computerized model. The conceptual model is composed of all the information, mathematical modeling data, and mathematical equations that describe the physical system or process of interest. The conceptual model is produced by analysis and observations of the physical system. In CFD, the conceptual model is dominated by the partial differential equations (PDEs) for conservation equations of mass, momentum, and energy. The computerized model is an operational computer program which implements a conceptual model. Modern terminology refers to the computerized model as the computer model or software. Figure 1 clearly depicts the meaning of verification and validation and their relationship to one another. To date, only Ref. [21] has recognized the value of exploring the concepts represented in Fig. 1 as they apply to verification and validation in computational simulation.

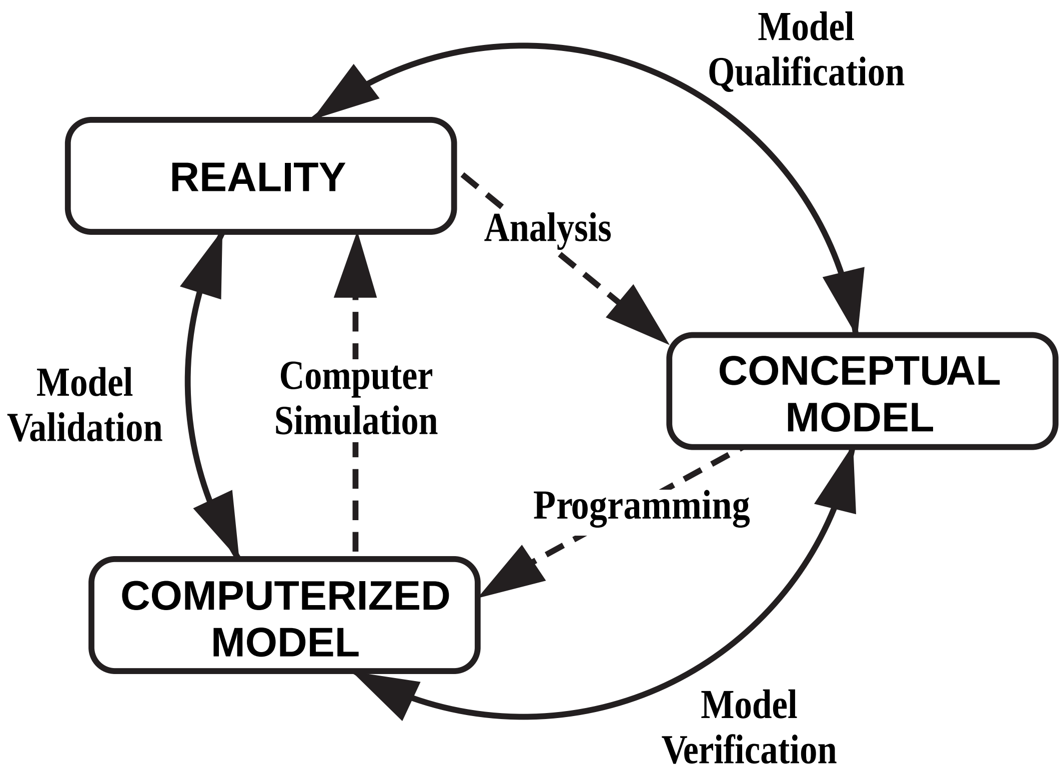

Figure 1
Phases of Modeling and Simulation [2]
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2.2 Verification and Validation

The definition of *verification* was taken from the DoD and modified slightly; whereas the definition of *validation* was taken verbatim from the DoD [3, 4]:

> *Verification*: The process of determining that a model implementation accurately represents the developer's conceptual description of the model and the solution to the model.
>
> *Validation*: The process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model.

As represented in Fig. 1, verification addresses the question of fidelity of the computational (or computerized) model to the conceptual model. We changed the DoD definition of verification to make it clear that the solution of the conceptual model is included in the accuracy determination. Validation addresses the issue of fidelity of the computational model, or its results, i. e., the simulation, to the real world. The term “Model Qualification” in Fig. 1 refers to the issue of fidelity of the conceptual model to reality. A term more consistent with the present work is “conceptual model validity” [12].

There are some important implications and subtleties in the definitions of verification and validation. The first key feature is that both are “process[es] of determining.” That is, they are ongoing activities that do not have a clearly defined completion point [4]. Completion or sufficiency is usually determined by practical issues such as budgetary constraints and intended uses of the model. The definitions include the ongoing nature of the process because of an unavoidable but distressing fact: the veracity, correctness, and accuracy of a CFD model cannot be demonstrated for all possible conditions and applications, except for trivial models. Trivial models are clearly not of interest. All encompassing proofs of correctness, such as those developed in mathematical analysis, do not exist in complex modeling and simulation. Indeed, nontrivial computer codes cannot be proven to be without error—much less models of physics. Only specific demonstrations of correctness or accuracy can be constructed in verification and validation activities.

The second feature that is common in the definitions of verification and validation is the stress on “accuracy,” which assumes that a measure of correctness can be determined. In verification activities, accuracy is generally measured with respect to benchmark solutions of simplified model problems. By benchmark solutions we mean either analytical solutions or highly accurate numerical solutions. In validation activities, accuracy is measured with respect to experimental data, i.e., reality. However, benchmark solutions and experimental data also have shortcomings. For example, benchmark solutions are extremely limited in the complexity of flow physics and geometry; and all experimental data have random and bias errors, which may cause the measurements to be *less* accurate than the CFD results. These issues are discussed in more detail in later sections of this document.

In essence, verification provides evidence that the model is solved right. Verification does not address whether the model has any relationship to the real world. Verification activities only evaluate whether the CFD model, which is the mathematical and computer software representation of the physical system, is solved accurately.

Validation, on the other hand, provides evidence that the right model is solved. This perspective implies that the model is solved correctly, or verified. Verification is the first step of the validation process and, while not simple, it is much less involved than the more comprehensive nature of validation. Validation addresses the question of the fidelity of the model to specific conditions of the real world. The terms “evidence” and “fidelity” both imply the concept of “estimation of tolerance;” not simply “yes” or “no” answers.

In simulations that involve complex flow physics or multidisciplinary engineering systems, strict validation procedures commonly become impractical. For example, when all of the required physical modeling parameters are not known a priori, some of the parameters must be determined using the experimental data. Or when grid-resolved solutions are not attainable because of the computer resources needed for the simulation, adjustments must be made to improve agreement with the experimental data. When these types of activities occur, the term *calibration* more appropriately describes the process than does validation. A definition of calibration is given in Section 4.2, where its relationship to validation is also discussed.

2.3 Uncertainty and Error

Uncertainty and error can be considered as the broad categories that are normally associated with loss in accuracy in modeling and simulation. A large body of research in many technical disciplines has addressed the identification and means of estimating a wide variety of uncertainties and errors. Some errors, like computer round-off and iterative convergence errors, are well understood. Some errors, such as the numerical error in the discrete solution of partial differential equations (PDEs) with singularities or discontinuities, are not well understood. Other shortcomings in modeling and simulation are associated with uncertainties rather than errors. Examples are the uncertainty in the surface roughness in the simulation of flow over a turbine blade and the uncertainty in the validity of a turbulence model.

In the CFD literature the terms uncertainty and error have commonly been used interchangeably [22-25]. It is believed, however, that failure to distinguish between these terms is detrimental to the quantification of credibility in modeling and simulation. This belief is strengthened by modern information theory, which has made significant progress in delineating the root causes and meaning of uncertainty [26, 27]. Some of the concepts advanced in modern information theory pertaining to the quantification of uncertainty have been applied by various researchers in the analysis of engineering system risk and failure [28-33]. Building on this literature, there has been a recent attempt to more carefully distinguish between uncertainties and errors in modeling and simulation [34]. The following definition of uncertainty is based on this recent work:

> *Uncertainty*: A potential deficiency in any phase or activity of the modeling process that is due to lack of knowledge.

The first feature stressed in the definition is *potential*, meaning that the deficiency may or may not occur. For example, there may be no deficiency in the prediction of some event, even though there is a lack of knowledge. Some type of probability distribution is commonly used to represent the occurrence or nonoccurrence of the deficiency. The second feature of uncertainty is that its fundamental cause is *lack of knowledge*. Lack of knowledge is commonly caused by incomplete knowledge of a physical characteristic or parameter as in the inadequate characterization of the distribution of surface roughness on a turbine blade. Lack of knowledge can also be caused by the complexity of a physical process like turbulent combustion, or by practical constraints on the level of detail used in a mathematical model of a physical process as in simplified models of turbulence.

There are two closely related methods for treating uncertainty: a sensitivity analysis and an uncertainty analysis [21, 23, 33, 35, 36]. A sensitivity analysis is composed of multiple simulations from a code to determine the effect of the variation of some component of the model, such as an input parameter or modeling assumptions, on certain output quantities. Sometimes sensitivity analyses are referred to as “what-if” or perturbation analyses. Sensitivity analyses, however, do not normally deal with the interaction of various uncertainty sources or the relative levels of confidence in variations. An example of a what-if sensitivity analysis is determining the effect of combustion chemistry models on the predicted thrust of a rocket engine. Like a sensitivity analysis, an uncertainty analysis is composed of multiple simulations; however, an uncertainty analysis is usually associated with the variability of a continuous model parameter that is properly represented by a probability distribution. An example of an uncertainty analysis is a Monte Carlo simulation to determine the effect of manufacturing variability of aluminum skin thickness on aeroelastic mode frequencies.

For error, we use the following definition [34]:

> *Error*: A recognizable deficiency in any phase or activity of modeling and simulation that is not due to lack of knowledge.

This definition stresses that the deficiency, or shortcoming, is identifiable or knowable upon examination. Thus there exists an agreed-upon approach that is considered to be more accurate, and it is practical to follow that approach. If divergence from the correct or more accurate approach is pointed out, the divergence is either corrected or allowed to remain. This implies a segregation of error types: errors can be either *acknowledged* or *unacknowledged*. Examples of acknowledged errors are round-off error in a digital computer, physical approximations made to simplify the modeling of a physical process, and a specified level of iterative convergence of a numerical scheme. When the analyst introduces these acknowledged errors into the modeling or simulation process, there are reasonable means of estimating the magnitude of the error introduced. Unacknowledged errors are blunders, or mistakes, commonly caused by people. For example, the analyst intended to do one thing in the modeling and simulation, but, due to human error, did another, e.g., a programming error. There are no straightforward methods for estimating or bounding the contribution of unacknowledged errors. The most common techniques for detecting unacknowledged errors are procedural methods; e.g., an independent check of input data reveals that a mistake was made.

These definitions distinguishing uncertainty and error may seem strange, or even inappropriate, to those familiar with experimental measurements. In experimental measurements, error is defined as [37] “the difference between the measured value and the true value.” Experimentalists define uncertainty as [37] “the estimate of error.” These definitions are inadequate for modeling and simulation for two reasons. First, the experimentalists’ definition of error depends on two factors; the measured value and the true value. The measured value is clear, but the true value is *not* known, except in the special case of comparison with a defined standard. For the general case then, the true value and the error are not known and they can only be subjectively estimated [30]. The definitions of error and uncertainty given here segregate the meaning of the two terms with knowledge, i.e., what is “known” (or can be ordered) and what is “unknown.” As a result, it can be seen that the definition of error given does not contradict the common meaning of error; the definition is simply less demanding. Second, by defining uncertainty as an estimate of error, the experimentalists are saying that, from the view of information theory, uncertainty and error are the same type of entity. For example, if the uncertainty were zero, then either the error would be zero, or the uncertainty would be erroneous.

2.4 Prediction and Levels of Credibility

This subsection describes the relationship between verification, validation, and prediction. In the context of verification and validation, the meaning of the word “prediction” should be restricted from its general usage to consider the history of validation activities with the CFD model.

> *Prediction*: Use of a CFD model to foretell the state of a physical system under conditions for which the CFD model has not been validated.

A prediction refers to the computational simulation of a specific case of interest that is *different* from cases that have been validated. This definition of prediction is a subset of the general meaning of prediction because it eliminates past comparisons with experimental data, i.e., it is a *pre*diction. If this restriction is not made, then there is little value in saying that one has reproduced agreement with experimental data. The stress on this meaning of prediction is made because modeling and simulation can be used in significantly different ways. By far the most common mode is to use computational simulation in cases for which we have a great deal of experience and closely related validation data. A second mode is characterized by the simulation of cases for which we have little experience and no related data. Between these two relatively extreme situations are varying degrees of experience and experimental data.

The processes of verification and validation should be viewed as historical statements, i.e., reproducible evidence that a model has achieved a given level of accuracy in the solution of specified problems. Viewed in this light, it becomes clear that the verification and validation processes do not directly make claims about the accuracy of predictions [4]. This explanation may seem contradictory to an intuitive understanding of these processes; or some may question the value of having a computational model verified and validated. The response to these views is two-fold. First, the accuracy of predictions from a computational model is not guaranteed by verification and validation processes because of the extraordinary nonuniqueness of the computational model. These processes *do not* address future usage of the code, for example, topics such as: correctness of the input parameters, accuracy of the new geometry of interest, appropriateness of the modeling assumptions, and the quality of grid generation. To better understand the nonuniqueness of the CFD model, consider the computational model as an exceptionally complex tool. By realizing that the computational model has thousands of configurations, each adjustable to particular situations, it becomes quickly apparent that how the tool is used is a major factor in its effectiveness. That is, the tool embodies such complexity that its proper use in future situations is clearly not unique or in any general sense “guaranteed.” Second, consider the situation where a computational model has completed some verification and validation process. Now the model is being used to compute a new flow field, such as a turbulent reacting flow that is different from the flow used in the test cases for verification and validation. One can then ask the fundamental question: “Given the verification and validation database, how can the accuracy of the new solution be estimated?” or similarly, “How can the credibility assurances of the verification and validation processes be quantified?” The answers to these questions are beyond the current state-of-the art in modeling and simulation.

Another important factor that affects the credibility of predictions is the level of complexity involved. There are three aspects of complexity in modeling and simulation that should be addressed: (1) the complexity of the physics, (2) the complexity of the model representing the physics, and (3) the level of prediction difficulty of an output quantity from the simulation [38]. Regarding the complexity of the physics modeling, fluid dynamics provides an extraordinarily wide range of complexity. The following categories provide one way of viewing the aspects of modeling complexity:

- Spatial dimensionality
- Temporal nature
- Geometry
- Flow physics

As one deals with these different aspects in a simulation, the credibility of the predictions is directly affected. If the simulation is restricted to a specific class of problems for which the CFD model has been verified and validated, then one’s confidence in the accuracy of the solution is clearly enhanced.

The second aspect of complexity concerns the level of modeling complexity. Different levels of physical modeling can give the same simulation accuracy because an increase in the level of modeling complexity *does not* necessarily increase the level of accuracy. As the level of complexity of the physics model increases, there is a corresponding increase in the number of sources of uncertainty and error, the quantity of information needed, and the computer resources required. There is a strong trend in CFD, particularly commercial CFD software, to maximize the comprehensiveness of software packages. However, the predictive power of a model depends on its ability to correctly identify the dominant controlling factors and their influences, not upon its completeness. A model of limited, but known, applicability is generally more useful, and less expensive to use, than a more complete model.

The third aspect of complexity is the level of prediction difficulty of the physical quantities of interest from the simulation. For example, validation of total body normal force on a hypersonic vehicle does not imply that surface heat flux from the simulation has been validated to the same degree of accuracy. The fidelity required to predict these two quantities is remarkably different. In many simulations some progressive order of prediction difficulty can be recognized. However, for complex multidisciplinary engineering systems this ordering becomes more formidable.

3. Verification Assessment

Verification is the process of determining that a model implementation accurately represents the developer's conceptual description of the model and the solution to the model. The fundamental strategy of verification is the identification and quantification of error in the computational model and its solution. As shown in Fig. 2, this process primarily relies on comparing the computational solution to the correct answer, which is provided by what we call “highly accurate solutions.”

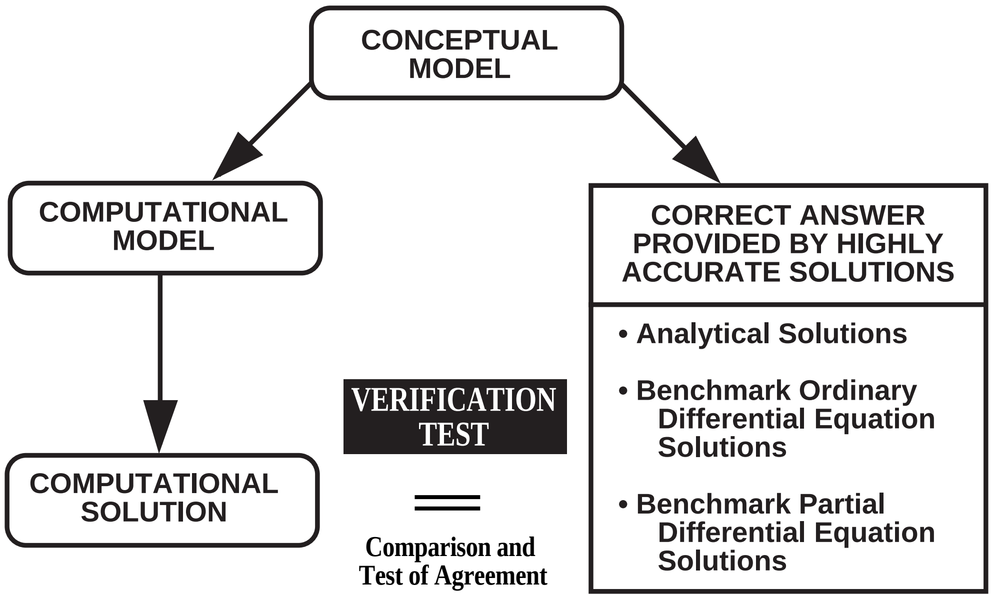

Figure 2
Verification Process

There are four predominant sources of error in CFD simulations: insufficient spatial discretization convergence, insufficient temporal discretization convergence, lack of iterative convergence, and computer programming. Section 3 contains procedures for identifying and estimating errors that may derive from these various sources and also a discussion about highly accurate solutions that can be used in measuring the accuracy of the computational solution. The procedures for estimating spatial, i.e., grid, and temporal convergence are similar and are presented together. Procedures for estimating iterative convergence include techniques for consistency checks on the solution. Programming errors are not addressed per se, but are referred to in the discussion about highly accurate solutions.

Verification activities are primarily performed early in the development cycle of a CFD code. However, these activities do need to be confirmed when the code is subsequently modified or enhanced. Although the required accuracy of the numerical solutions obtained during verification activities depends on the problem and the intended uses of the code, the accuracy requirements in verification activities are generally more stringent than the accuracy requirements in validation activities. The guidelines presented in this section apply to finite difference, finite volume, and finite element procedures. Procedures for other numerical approaches, such as vortex methods, lattice gas methods, and Monte Carlo methods are not addressed.

3.1 Grid and Time-Step Convergence

The most important activity in verification testing is systematically refining the grid size and time step. The objective of this activity is to estimate the discretization error of the numerical solution. As the grid size and time step approach zero, the discretization error should monotonically approach zero, excluding computer round-off errors. This relationship occurs because the defining characteristic in this monotonic region is that the order of accuracy of the discretized equations being solved is constant as the grid and time step are reduced. When the monotonic region has been demonstrated, Richardson's extrapolation can be used to estimate zero-grid spacing and time step [23, 24, 39-42]. At this point, the numerical scheme is said to be both grid and time-step convergent. Because this definition of convergence typically demands a large amount of computer resources, it is usually applied on simplified or model problems. The more common, but not rigorous, meaning of convergence is that little change in important dependent variables can be observed during grid and time-step refinement. It should also be noted that grid and time-step refinement often exposes discretization errors and programming errors.

Generally, second-order accurate difference schemes as a minimum should be employed in any computational procedure. Neumann-type boundary conditions should be discretized to the same order of accuracy as points in the interior of the domain. The second-order nature of a given solution is exhibited by the fact that the discretization error decreases by a factor of four when the grid size is halved. For complex flow fields, it is commonly found that insufficient grid resolution is used on the first two solutions such that higher-order terms in Richardson's extrapolation are not negligible. Until the computed grid convergence rate from two individual solutions, with the same grid clustering, matches the known (or previously demonstrated) order of accuracy of the code, Richardson's extrapolation cannot be used to estimate error [40, 43]. If Richardson's extrapolation method is validated using three different grid resolutions, then an estimate can be made of the grid-resolved solution variable. Similar comments apply to time-step reduction. Grid convergence rates can depend on other factors such as local flow characteristics and grid clustering. For example, it is much harder to converge to an accurate solution in regions where variables such as velocity and temperature vary rapidly through a boundary layer or free shear layer. Grid convergence rates can also depend on the relevant dimensionless parameters of the flow, such as Reynolds number and Mach number, and considerations such as the turbulence model used.

Richardson's extrapolation applies not only to computed dependent variables at all grid points, but also to solution functionals. Solution functionals are integrated and differentiated quantities such as body lift and surface heat flux, respectively. Different dependent variables and functionals converge at different rates. For example, the grid and time step required to show second-order convergence in local surface heat flux are typically much finer than for total lift on a body. A Grid Convergence Index (GCI), based on Richardson's extrapolation, has been developed to aid in estimating grid convergence error [24, 44]. The GCI converts error estimates obtained from any grid refinement ratio into an equivalent grid-doubling estimate.

Singularities and discontinuities pose an especially difficult task for verification. By definition, the discretization is not valid because higher-order derivatives that are neglected in the Taylor series expansion are not small. When possible, singularities caused by the geometry or the coordinate system should be removed by suitable mathematical transformation. Singularities inherent in the conceptual model should be removed by including the suitable physical information that was left out of the discretized model. In problems where the singularity cannot be removed and in flows with discontinuities, it is to be expected that local grid and time-step refinement may not lead to a fully grid-resolved solution. For such problems, the results of the local grid and time-step refinement should be presented, and the extent of the influence of the singularity and discontinuity on grid and time-step refinement elsewhere in the flow should be documented.

3.2 Iterative Convergence and Consistency Tests

In most cases CFD equations are highly nonlinear, and the vast majority of methods of solving these equations require iteration. These iterations normally occur in two situations: 1) globally, i.e, over the entire domain, for boundary value problems; and 2) within each time step for initial-boundary value problems. Often an iterative convergence tolerance is specified, and the difference between the solution of successive iteration steps at each point in the grid is computed. If the magnitude of this difference is less than the specified tolerance, then the numerical scheme is said to iteratively converge. The absolute-value tolerance test, however, is not recommended because the tolerance value is not scaled with respect to the values being tested. All iterative-convergence tolerance criteria should be scaled by the magnitude of the values tested; that is, a relative error criterion should be used. Scaling, however, should not be done when the value is zero or the value has no meaningful precision because of computer round-off. In verification testing, the sensitivity of the solution to the magnitude of the convergence criteria should be varied and a value should be established that is consistent with the objectives of the simulation. It should be realized that such convergence criteria, both absolute and relative errors, depend on the rate of convergence of the iterative scheme.

For boundary value problems, a more reliable technique of determining iterative convergence is to base the criteria on the residual error remaining in the difference equation [45]. A residual vector is computed for each iteration, i. e., the error in the present solution iteration as compared to the exact solution of the difference equations. To measure the residual error over the entire domain, an appropriate vector norm is computed. This value is then compared with the magnitude of the residual error at the beginning of the iteration. When the error norm decreases by, say, five orders of magnitude, one can more confidently determine iterative convergence. This error norm can be computed for any or all of the dependent variables in the system of PDEs. This technique of computing the residual error is applicable to a wide variety of iterative methods and its reliability is not dependent on the rate of convergence of the numerical scheme.

For unsteady flow problems, the solution is usually obtained by marching in time and globally solving in space at each time step. The iterative procedure is similar at each time step; however, since time-step error is cumulative, iteration errors can accumulate and destroy the integrity of the solution. For an unsteady flow problem, the values of relative per-step convergence criteria should be at least an order of magnitude smaller than the global convergence criteria for a steady flow problem.

Various other checks, which are termed consistency checks, can be also be employed in verification testing. Global checks on conservation of appropriate quantities can be made [46], as well as checks with regard to the effect of the boundary conditions on the solution. One group of boundary condition tests evaluates whether certain symmetry features are preserved in the solution. For example, if a plane of symmetry exists in the conceptual model, then the normal gradient of appropriate variables can be set to zero and a solution obtained. The same solution should also be obtained if this plane of symmetry condition is not imposed and the entire flow field is solved. In external flow fields, the boundaries of the computational domain are conceptually considered to be at infinity, i. e., they are far from the spatial region of interest. Typically, a user-defined parameter specifies how "far out" these boundaries are. If the boundaries are too close, the asymptotic conditions applied there may not be accurate. The usual method of determining the size of the computational domain is to systematically increase the domain until the solution is no longer dependent on the size of the domain consistent with the objectives of the computation. It is important to note that this exercise must be performed for a suitable grid and time step that are within the grid and time-step convergence envelope.

3.3 Highly Accurate Solutions

Comparing a computational solution to a highly accurate solution is the most accurate and reliable way to quantitatively measure the error in the computational solution. However, highly accurate solutions are known only for a relatively small number of simplified problems. These highly accurate solutions can be classified into three types identified previously in Fig. 2: analytical solutions, benchmark numerical solutions to ordinary differential equations (ODEs), and benchmark numerical solutions to the PDEs.

Analytical solutions refer to closed-form solutions to special cases of the PDEs represented in the conceptual model. These closed-form solutions are commonly represented by infinite series, integrals, and asymptotic expansions [47-54]. As a result, numerical methods are usually used to compute the solutions of interest. However, the accuracy of these solutions can be quantified much more rigorously than numerical solutions of the conceptual model. The most significant practical shortcoming of analytical solutions is that they exist for only very simplified physics and geometries. A technique for generating a wider variety of analytical solutions for verification activities has also received attention [55, 56]. These analytical solutions, however, are solutions to PDEs that are very similar to the equations of fluid dynamics, but with additional terms.

When computational solutions are compared with highly accurate solutions, the comparisons should be examined along boundaries of interest or error norms computed over the entire solution domain. The accuracy of each of the dependent variables or functionals of interest should be determined. As previously noted, the required fidelity of the numerical solution varies greatly with the type of solution variable computed.

Benchmark ODE solutions are very accurate numerical solutions to special cases of the general CFD model. These ODEs commonly result from simplifying assumptions, such as simplified geometries and assumptions that result in the formation of similarity variables. Examples are the Blasius solution for laminar flow over a flat plate, the Taylor-Maccoll solution for inviscid flow over a sharp cone, and the stagnation-region flow in two dimensions and three dimensions [49-51, 53].

Benchmark PDE solutions are also very accurate numerical solutions to special cases of either the PDEs, or special cases of the boundary conditions. Examples of various benchmark PDE solutions are the following: incompressible laminar flow over a semi-infinite flat plate [57-59], incompressible laminar flow over a parabolic plate [60-62], incompressible laminar flow in square cavity driven by a moving wall [63-70], laminar natural convection in a square cavity [71, 72], incompressible laminar flow over an infinite-length circular cylinder [73-76], and incompressible laminar flow over a backward-facing step, with and without heat transfer [77-81]. (Note that we have not attempted to list all of the high quality solutions of these flow fields, but only representative solutions.) As one moves from ODE solutions to PDE solutions, the accuracy of the benchmark solutions clearly becomes more of an issue. Indeed, the literature has examples of flow field calculations that are considered to be of high accuracy by the author, but later are found to be lacking. This guide recommends that no published solution be considered as a benchmark solution until it has been calculated very carefully by independent investigators, preferably using different numerical approaches.

4. Validation Assessment

Validation is the process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model. The fundamental strategy of validation is the identification and quantification of error and uncertainty in the conceptual and computational models. Since the primary role of CFD in engineering is to serve as a high-fidelity tool for design and analysis, it is essential to develop a systematic, rational, and affordable code validation process that is applicable to a wide variety of engineering applications. The process recommended in this guide is depicted in Fig. 3. The method of measuring the accuracy of the representation of the real world is achieved by systematically comparing CFD simulations with experimental data. This does not imply that experimental data has perfect accuracy. All experimental data contain bias errors and random errors. The estimate of the magnitude of these errors, i.e, experimental uncertainty, must be included in the comparison with the computational simulations.

During validation assessment activities, there are several practical issues that should be considered:

1. The number of validation test cases and the accuracy level required for each test case are highly application-dependent. It is not possible to define a single set of criteria for all applications.

2. Very high accuracy in engineering calculations, while highly desirable, is not essential since most design changes are incremental over a baseline. As long as the trends predicted by the tools are consistent within the design envelope and an estimate of the error and uncertainty can be made, less-than-perfect accuracy of the simulation is commonly acceptable.

3. The validation process must be realistically achievable within an engineering environment, where there may be significant pressure to apply a code and produce results before validation is complete. The engineering environment implies computational robustness over a range of physical and numerical parameters.

Thus the validation process must be flexible, must allow for varying levels of accuracy, and must be tolerant of incremental improvements as time and funding permit.

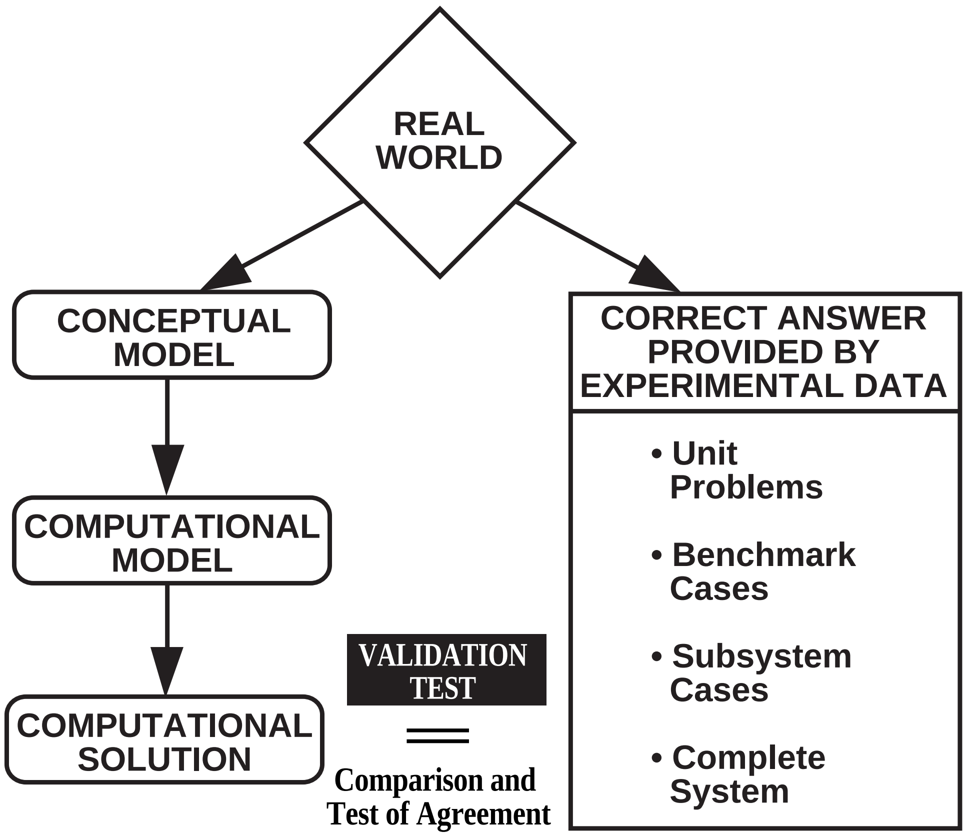

Figure 3
Validation Process

4.1 Validation Phases

Several validation methods have been suggested, but most of these are tentative or have not been developed in depth. The recommended method is to employ a building-block approach [82-86], as shown in Fig 4. This approach divides the complex engineering system of interest into three progressively simpler phases: subsystem cases, benchmark cases, and unit problems. The strategy in this approach is the assessment of how accurately the computational results compare with experimental data (with quantified uncertainty estimates) at multiple levels of complexity.

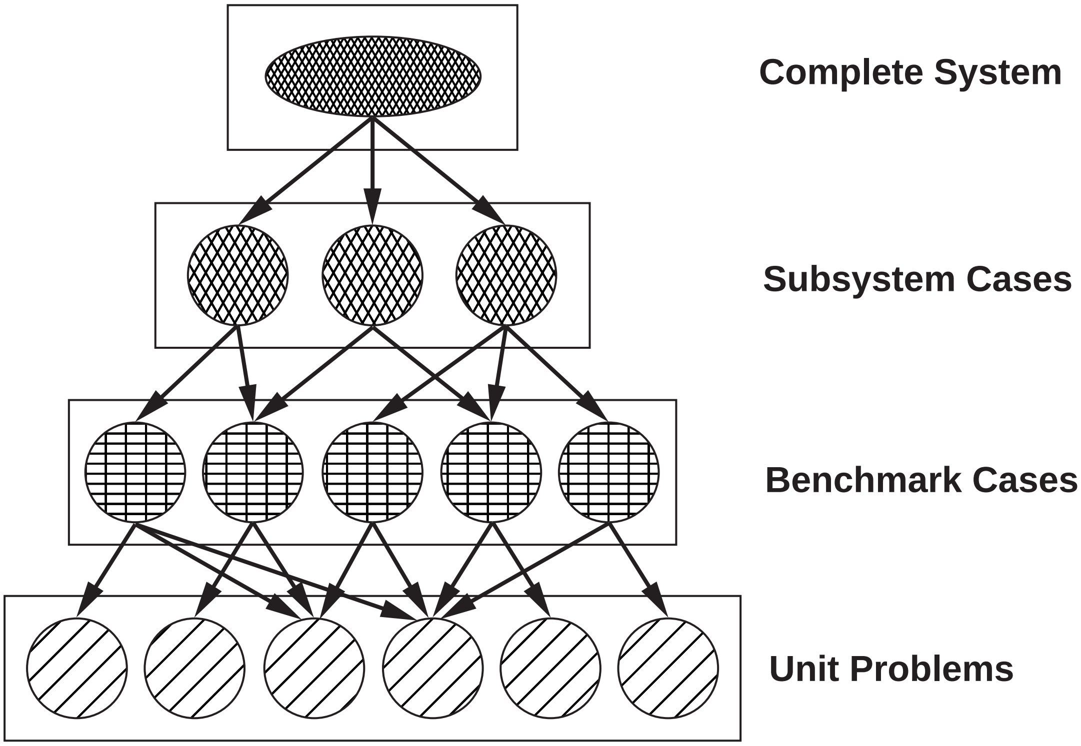

Figure 4
Validation Phases [85]

Each phase of the process represents a different level of flow physics coupling and geometrical complexity (see Fig. 5). The complete system consists of the actual hardware or system for which a validated CFD tool is needed. Thus, by definition, all the geometric and flow physics effects occur simultaneously; commonly, the complete system includes multidisciplinary physical phenomena. Data are measured on the engineering hardware under realistic operating conditions. These measurements, however, are very limited. Exact test conditions, e.g., initial conditions (ICs) and boundary conditions (BCs), are hard to quantify; and the data are generally of engineering quality with a fairly high degree of uncertainty.

Subsystem cases represent the first decomposition of the actual hardware into simplified or partial flow paths. Each of these cases commonly exhibits restricted geometric or flow features compared to the complete system. The flow physics of the complete system may be reasonably well represented by these subsystem cases, but the level coupling between flow phenomena is typically reduced. The quality and quantity of the test data are usually significantly better than the complete system.

Benchmark cases represent another level of successive decomposition of the complete system. For these cases, separate hardware is fabricated to represent key features of each subsystem. The benchmark cases are geometrically simpler than those at the subsystem level, and only two separate features of the flow physics and two flow features are commonly coupled in the benchmark cases. Examples of coupled flow features are: boundary layer separation caused by a shock wave, the interaction of cavitating flow with a separated flow region, and ignition of a combustible mixture caused by a shock wave. The experimental data obtained in this phase are usually well documented and are quite extensive in scope. Most of the experimental uncertainties associated with the measurements are quantified, but some important measurements may be missing, e.g., some initial and boundary conditions.

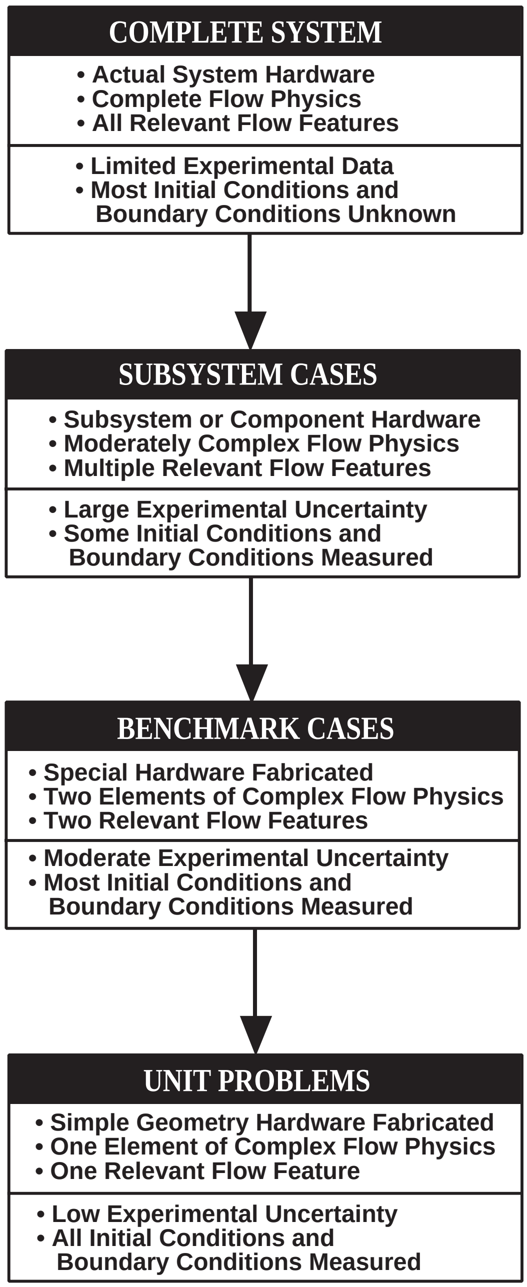

Figure 5
Characteristics of Validation Phases

Unit problems represent the total decomposition of the complete system. High-precision, special-purpose hardware is fabricated and inspected. Unit problems are characterized by very simple geometries, one flow-physics feature, and one dominant flow feature. Highly instrumented, highly accurate experimental data are obtained. In addition, an extensive uncertainty analysis of the experimental data is prepared. Commonly, experiments on unit problems are conducted at separate facilities to ensure identification of bias, or systematic, errors in the experimental data. For unit problems, all important boundary conditions and initial conditions are accurately measured.

Each phase of the validation process emphasizes the assessment of certain features of the CFD model. For unit problems, all numerical aspects of the code are exercised to verify accuracy, functionality, and iterative convergence characteristics. Additionally, systematic grid sensitivity studies are conducted to assess grid convergence error and to provide guidance in specifying computational grid clustering for more complex flow cases. For benchmark cases, the emphasis shifts to assessing the physical models in the code given the limited coupling of physics in this phase. Grid sensitivity studies are also conducted to assess the level of refinements necessary to capture key physical effects. Lessons learned from unit problems are used to guide the benchmark case activities. Overall, fewer cases are run in the benchmark-case phase than in the unit-problems phase. For subsystems, the strategy is to exercise the complete code on flow cases that contain multiple geometric and flow features similar to these found in the complete system. The effects of grid topology and local grid clustering, as well as the physical modeling requirements with strong coupling, are determined at this phase. Relatively few cases are run. For the complete system, the most appropriate physical models, the best grid topology, and grids that are appropriately refined and clustered are used to simulate the actual hardware test case(s). The level of agreement achieved with the test data (taking into account measurement uncertainties) is then reviewed in light of the design accuracy requirements to establish the level of code validation for that application category.

The validation process described above should create, over time, an extensive validation database that can be used to guide future designs without having to repeat all the validation phases. As a CFD code is validated to different levels for a given application, a knowledge database is developed and gradually extended. Therefore, extending an existing validation effort to either the next level or to a related application becomes relatively straightforward, since comparatively few cases may need to be validated. An example of this approach is given in Fig. 6. Here the validation of a code to analyze a turbopump impeller-diffuser interaction problem also provides a validated code, up to the subsystems level, for the analysis of blade-cracking problems in a turbine.

4.2 Calibration

The quantification of prediction increments is the most common use of modeling and simulation in engineering. This conservative approach provides incremental changes in complex systems and processes so that a wide variety of modeling and simulation shortcomings can be tolerated without unacceptable risk. For example, the difference between the design expectation and actual performance of a fluid dynamics system, say an aircraft or a turbopump, is a measure of the uncertainty and error inherent within the simulation. Once the uncertainty and error have been estimated, the same design simulation tools are used in the same manner to estimate the performance

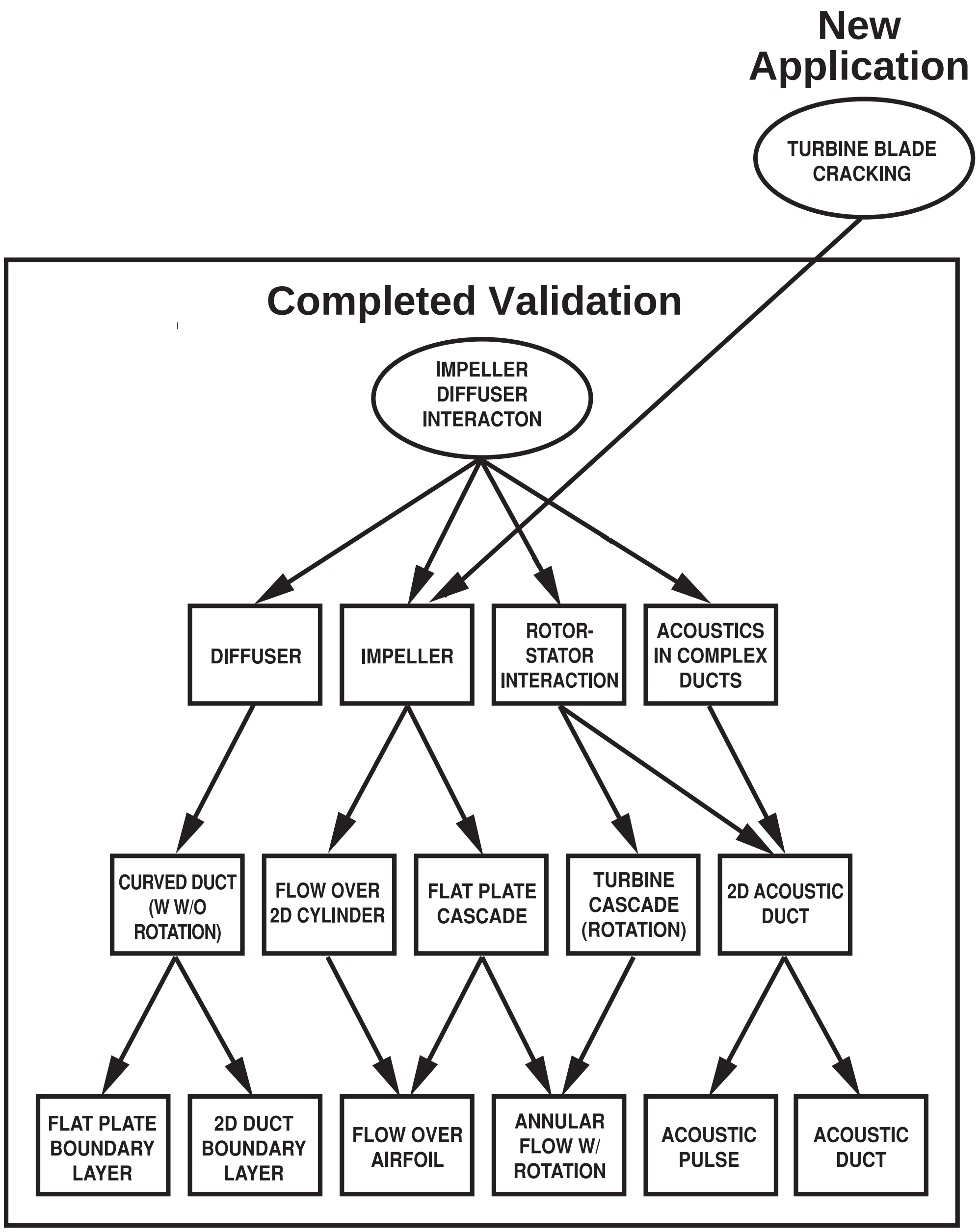

Figure 6
Use of Completed Validation Cases for New Applications [85]

of other similar systems operating in a comparable environment. This is commonly done either by adding the known uncertainty and error to the simulated performance value, or by adjusting for various elements of the simulation so that the computational results agree with the measured results. Adjustment activities are commonplace in complex CFD simulations and are conceptually different from activities associated with the validation process. In effect, such activities comprise a different process, which we refer to by the term *calibration*.

> *Calibration*: The process of adjusting numerical or physical modeling parameters in the computational model for the purpose of improving agreement with real-world data.

Calibration is *not* "the process of determining the degree to which a model is an accurate representation of the real world." Calibration is primarily directed toward improving agreement of computational results with existing experimental data, *not* determining the accuracy of the results. Because of constraints in fiscal budgets and computer resources, or because of incomplete physical modeling data, calibration is commonly an appropriate process when compared to validation. The distinction between calibration and validation is not always crisp or easily recognizable in many situations. However, attempts should be made to recognize when calibration is exercised because it directly impacts the confidence in predictions from the CFD model. Stated differently, calibration affects "how far" from the existing experimental database one can make a prediction and still retain an acceptable level of confidence in the prediction. Calibration does not generate the same level of predictive confidence as validation.

The need for calibration commonly arises when there is uncertainty in the modeling of complex physics processes and also when there is incomplete or imprecise characterization of experiments. Situations in which physical modeling parameters are commonly adjusted are found in the computation of turbulent combusting flow, multiphase flows, and flows with strong coupling to other physical processes, such as acoustics, structural dynamics, and radiation transport. For example, consider the use of the Reynolds-Averaged Navier Stokes equations in computing turbulent reacting flow with finite rate chemistry. It is common practice to adjust chemical reaction rates so that improved agreement with experimental data is obtained. Another example is the adjustment of unmeasured or poorly characterized experimental parameters, e.g., boundary conditions, in comparisons of computations with experiment data. Incomplete or imprecise experimental data are often viewed as adjustable parameters by the code user when making comparisons with experimental data. This type of physical parameter adjustment activity is similar to the highly developed technique of parameter identification used in many other disciplines. For example, in structural dynamics, mechanical joint stiffness and joint damping are clearly identified as physical modeling parameters that are optimally estimated in simulation comparisons with experimental measurements of structural modes. Formal parameter identification procedures clearly recognize the calibration nature of the analysis.

How CFD calibration activities impact confidence in predictions, i.e., the accuracy of future computational results, is very difficult to determine and is presently beyond the state-of-the-art. Similarly, the issue of assessing the accuracy of predictions is usually complicated by the lack of grid or time-step convergence in the calibration computations. It is common engineering practice to use the results of CFD simulations for complete systems and subsystems applications for which grid-resolved solutions are not attained–possibly far from being resolved. Indeed, benchmark cases and even unit problems with complex physics, particularly three-dimensional simulations, may not have grid-resolved solutions. When physical modeling parameters are determined based on solutions on grids that are clearly under-resolved, the activity should be considered as part of the calibration. The calibration nature of this type of activity is recognized if the physical modeling parameters are readjusted based on solutions obtained on finer grids. The calibration nature of such an activity should also be recognized if grid refinement is stopped when generally good agreement is obtained with the important experimental measurements; in other words, if further refined grids show degraded agreement with the experimental data.

As mentioned earlier in this section, some of the subtleties of calibration as compared to validation are highlighted in order to further the understanding of each process. Also, improved understanding of calibration and validation will aid in developing future methods for quantitatively estimating confidence in predictions for complex systems.

4.3 Requirements for Experimental Data

Recently, there have been increased efforts directed toward improving methods for quantifying uncertainty in experimental measurements [87, 88]. These efforts should aid in obtaining the appropriate data needed for each phase of the validation process. Experimental data from complete systems and data from subsystem tests are always hardware-specific and are available mainly through large-scale test programs. The amount of data provided for these phases is generally limited to engineering parameters of design interest and system performance measures. The data may have large uncertainty bands, or there may have been no attempt to estimate uncertainty. These test programs typically require expensive ground test facilities, or they are full-scale flight test programs. The test programs are also commonly conducted under hostile environmental conditions with rigid budget and schedule constraints. Consequently, the complete set of required physical modeling parameters, boundary conditions, and initial conditions needed for validation assessment is never obtained. Indeed, it is often impractical or even impossible with current technology to obtain all of the required information.

Benchmark cases and unit problems should provide the quantity and quality of data required for precise code validation. These two phases should be considered as true CFD model validation experiments because all of the important activities are performed for the primary purpose of validation, with little regard for system or subsystem performance, reliability, or product competition issues. A summary of guidelines for a validation experiment methodology follows [89-92]:

1. A validation experiment should be jointly designed by experimentalists and CFD code developers or users working closely together throughout the program, from inception to documentation, with complete candor as to the strengths and weaknesses of each approach.

2. A validation experiment should be designed to capture the essential flow physics, including all relevant physical modeling data and initial and boundary conditions required by the code.

3. A validation experiment should strive to emphasize inherent synergism between computational and experimental approaches.

4. Although the experimental design should be developed cooperatively, complete independence must be maintained in obtaining both the computational and experimental results.

5. A hierarchy of experimental measurements of increasing difficulty and specificity should be made, for example, from globally integrated quantities to local flow measurements.

6. An uncertainty analysis procedure should be employed that delineates and quantifies systematic and random error sources by type.

In general, validation data for benchmark cases and unit problems should not be company-proprietary or restricted for security reasons. These data should be compiled in publicly available databases, like the European hypersonic database [93], and others [94-98]. The need for quality data appropriate for CFD validation cannot be overemphasized.

5. Summary and Conclusions

One of the primary factors in the rate of growth of CFD as a research and engineering tool in the future will be the level of credibility that can be developed in the simulations produced. The CFD Committee on Standards strongly believes that the key to building this credibility is the development of commonly accepted and applied verification and validation terminology and methodology. As defined here, verification is the process of determining the accuracy of a given computational solution; that is, has the problem been solved correctly? The fundamental strategy of verification is the identification and quantification of error in the computational solution. Validation is the process of assessing the degree to which the computational simulation represents the real world; that is, has the correct problem been solved? The fundamental strategy of validation is the identification and quantification of error and uncertainty in the mathematical model of the physics and computational solution. Other foundational terms include uncertainty, error, prediction, and calibration. This document attempts to provide a foundation for the major issues and concepts in verification and validation.

These guidelines are predicated upon the notion that there is no fixed requirement of accuracy that is applicable to all CFD simulations. The accuracy level required of simulations depends on the purposes for which the simulations are to be used. Not all simulations need to demonstrate high accuracy as long as the error and uncertainty of the simulations can be estimated. In CFD simulations of complex engineering systems, the accuracy level is influenced by such factors as cost, schedule, and risk of the failure of the system.

It has been emphasized that the methodology presented in this document provides guidelines, not performance requirements. The CFD Committee on Standards believes that the state-of-the-art in CFD has not developed to the point where conformity can be required. For example, much more research needs to be conducted toward improving the detailed methodology and procedures of verification and validation. In addition, research is needed into mathematical methods for the quantitative assessment of confidence in predictions based on verification and validation activities.

6. REFERENCES

1. Tannehill, J. C., Anderson, D. A., and Pletcher, R. H., *Computational Fluid Dynamics and Heat Transfer,* Taylor & Francis, Washington, DC, 1997.

2. Schlesinger, S., "Terminology for Model Credibility," *Simulation*, Vol. 32, No. 3, 1979, pp. 103-104.

3. DoD, "DoD Instruction 5000.61: Modeling and Simulation (M&S) Verification, Validation, and Accredization (VV&A)," Defense Modeling and Simulation Office, Office of the Director of Defense Research and Engr., available: www.dmso.mil/docslib, April 29, 1996.

4. DoD, "Verification, Validation, and Accreditation (VV&A) Recommended Practices Guide," Defense Modeling and Simulation Office, Office of the Director of Defense Research and Engr., available: www.dmso.mil/docslib, Oct. 28, 1996.

5. ASME-JFE, "Journal of Fluids Engineering Editorial Policy Statement on the Control of Numerical Accuracy," *Journal of Fluids Engineering*, Vol. 115, No. 3, 1993, pp. 339-340.

6. AIAAJ, "Editorial Policy Statement on Numerical Accuracy and Experimental Uncertainty," *AIAA Journal*, Vol. 32, No. 1, 1994, pp. 3.

7. ASME-JHT, "Editorial Policy Statement on Numerical Accuracy," *Journal of Heat Transfer,* Vol. 116, No. 11, 1994, pp. 797-798.

8. IJNMF, "Editorial," *International Journal of Numerical Methods in Fluids*, Vol. 19, No. 12, 1994, pp. iii.

9. Conway, R. W., "Some Tactical Problems in Digital Simulation," *Management Science*, Vol. 10, No. 1, 1963, pp. 47-61.

10. Naylor, T. H., and Finger, J. M., "Verification of Computer Simulation Models," *Management Science,* Vol. 14, No. 2, 1967, pp. 92-101.

11. Naylor, T. H., *Computer Simulation Experiments with Models of Economic Systems*, Wiley, New York, 1971.

12. Sargent, R. G., "An Expository on Verification and Validation of Simulation Models," *1985 Winter Simulation Conference*, Sacramento, CA, 1985.

13. Balci, O., and Nance, R. E., "Formulated Problem Verification as an Explicit Requirement of Model Credibility," *Simulation*, Vol. 45, No. 2, 1985, pp. 76-86.

14. Law, A. M., and Kelton, W. D., *Simulation Modeling and Analysis*, 2nd ed, McGraw-Hill, New York, 1991.

15. IEEE, "IEEE Standard Glossary of Software Engineering Terminology," IEEE, IEEE Std 610.12-1990, New York, NY, Feb. 1991.

16. Knepell, P. L., and Arangno, D. C., *Simulation Validation: A Confidence Assessment*, 1st ed, IEEE Computer Society Press, Washington, 1993.

17. ANS, "American Nuclear Society: Guidelines for the Verification and Validation of Scientific and Engineering Computer Programs for the Nuclear Industry," ANSI/ANS-10.4-1987, 1987.

18. ISO, "International Standard ISO 9000-3: Quality Management and Quality Assurance Standards - Part 3: Guidelines for the application of ISO 9001 to the development, supply and maintenance of software," International Standards Org., 1991.

19. Schmauch, C. H., *ISO 9000 for Software Developers*, ASQC Quality Press, Milwaukee, WI, 1994.

20. Neelamkavil, F., *Computer Simulation and Modelling*, 1st ed, John Wiley & Sons, New York, 1987.

21. Mehta, U. B., "Guide to Credible Computer Simulations of Fluid Flows," *Journal of Pro-*

pulsion and Power, Vol. 12, No. 5, 1996, pp. 940-948.

22. Mehta, U. B., "Some Aspects of Uncertainty in Computational Fluid Dynamics Results," *Journal of Fluids Engineering*, Vol. 113, 1991, pp. 538-543.

23. Celik, I., and Zhang, W. M., "Calculation of Numerical Uncertainty Using Richardson Extrapolation: Application to Some Simple Turbulent Flow Calculations," *Journal of Fluids Engineering*, Vol. 117, 1995, pp. 439-445.

24. Roache, P. J., "Quantification of Uncertainty in Computational Fluid Dynamics," in *Annual Review of Fluid Mechanics,* Annual Reviews, Inc., 1997, pp. 126-160.

25. Lotz, R. D., Thompson, B. E., Konings, C. A., and Davoudzadeh, F., "Numerical Uncertainties in Transonic Flow Calculations for Aerofoils with Blunt Trailings Edges," *International Journal of Numerical Methods in Fluids,* Vol. 24, No. 4, 1997, pp. 355-373.

26. Klir, G. J., and Folger, T. A., *Fuzzy Sets, Uncertainty, and Information*, 1st ed, Prentice Hall, Englewood Cliffs, NJ, 1988.

27. Almond, R. G., *Graphical Belief Modeling*, 1st ed, Chapman & Hall, London, U. K., 1995.

28. Ditlevsen, O., *Uncertainty Modeling with Applications to Multidimensional Civil Engineering Systems*, 1st ed, McGraw-Hill, Inc., New York, NY, 1981.

29. Beck, M. B., "Water Quality Modeling: A Review of the Analysis of Uncertainty," *Water Resources Research*, Vol. 23, No. 8, 1987, pp. 1393-1442.

30. Morgan, M. G., and Henrion, M., *UNCERTAINTY A guide to Dealing with Uncertainty in Quantitative Risk and Policy Analysis*, 1st ed, Cambridge University Press, New York, 1990.

31. Ayyub, B. M., Gupta, M. M., and Kanal, L. N., eds. *Analysis and Management of Uncertainty: Theory and Applications*, 1st ed. 1992, North-Holland, New York.

32. Ayyub, B. M., and Gupta, M. M., eds. *Uncertainty Modelling and Analysis: Theory and Applications*, 1st ed. 1994, North-Holland, New York.

33. McKay, M. D., "Aspects of Modeling Uncertainty and Prediction," Los Alamos National Labs., 94-605, Los Alamos, NM, 1994.

34. Oberkampf, W. L., Diegert, K. V., Alvin, K. F., and Rutherford, B. M., "Variability, Uncertainty, and Error in Computational Simulations," ASME Paper No. 25.1, *ASME/AIAA Joint Thermophysics and Heat Transfer Conference*, Albuquerque, NM, 1998.

35. Mehta, U. B., "Computational Requirements for Hypersonic Flight Performance Estimates," *Journal of Spacecraft and Rockets*, Vol. 27, No. 2, 1990, pp. 103-112.

36. Cribbs, D. W., "Performance Uncertainty Analysis for NASP," AIAA Paper No. 90-5209, Orlando, FL, 1990.

37. Coleman, H. W., and Steele, W. G., Jr., *Experimentation and Uncertainty Analysis for Engineers*, 1st ed, John Wiley & Sons, New York, 1989.

38. Oberkampf, W. L., "A Proposed Framework for Computational Fluid Dynamics Code Calibration/Validation," AIAA Paper No. 94-2540, *18th AIAA Aerospace Ground Testing Conference*, Colorado Springs, CO, 1994.

39. Richardson, L. F., and Gaunt, J. A., "The Deferred Approach to the Limit," *Transactions of the Royal Society of London, Series A: Mathematical and Physical Sciences*, Vol. 226, 1927, pp. 299-361.

40. Fletcher, C. A. J., *Computational Techniques for Fluid Dynamics*., Vol. 1, Springer-Verlag, New York, 1988.

41. Blottner, F. G., "Accurate Navier-Stokes Results for the Hypersonic Flow Over a Spherical Nosetip," *Journal of Spacecraft and Rockets*, Vol. 27, No. 2, 1990, pp. 113-122.

42. Zingg, D. W., "Grid Studies for Thin-Layer Navier-Stokes Computations of Airfoil Flowfields," *AIAA Journal*, Vol. 30, No. 10, 1992, pp. 2561-2564.

43. Oberkampf, W. L., and Blottner, F. G., "Issues in Computational Fluid Dynamics Code Verification and Validation," Sandia National Labs., SAND95-1352, Albuquerque, NM, Sept. 1997.

44. Roache, P. J., "Perspective: A Method for Uniform Reporting of Grid Refinement Studies," *Journal of Fluids Engineering*, Vol. 116, 1994, pp. 405-413.

45. Axelsson, O., *Iteative Solution Methods,* Cambridge Univ. Press, Cambridge, 1996.

46. Haworth, D. C., Tahry, S. H. E., and Huebler, M. S., "A Global Approach to Error Estimation and Physical Diagnostics in Multidimensional Computational Fluid Dynamics," *International Journal for Numerical Methods in Fluids*, Vol. 17, 1993, pp. 75-97.

47. Karamcheti, K., *Principles of Ideal-Fluid Aerodynamics*, Wiley, New York, 1973.

48. Nayfeh, A. H., *Perturbation Methods*, Wiley, New York, 1973.

49. Hayes, W. D., and Probstein, R. F., *Hypersonic Flow Theory: Vol. 1 Inviscid Flows*, Academic Press, New York, 1966.

50. Panton, R. L., *Incompressible Flow*, Wiley, New York, 1984.

51. Wang, C. Y., "Exact Solutions of the Steady-State Navier-Stokes Equations," in *Annual Review of Fluid Mechanics*, J.L. Lumley and M.V. Dyke, Editors, Annual Reviews, Inc., Palo Alto, CA, 1991, pp. 159-177.

52. Ethier, C. R., and Steinman, D. A., "Exact Fully 3D Navier-Stokes Solutions for Benchmarking," *International Journal for Numerical Methods in Fluids*, Vol. 19, 1994, pp. 369-375.

53. Wilcox, D. C., *Perturbation Methods in the Computer Age*, DCW Industries, La Canada, CA, 1995.

54. Grenda, J. M., Schwer, D. A., and Merkle, C. L., "Use of Analytical Solutions in Validating Unsteady CFD Codes," *1st AIAA Theoretical Fluid Mechanics Meeting*, New Orleans, LA, AIAA, 1996.

55. Steinberg, S., and Roache, P. J., "Symbolic Manipulation and Computational Fluid Dynamics," *Journal of Computational Physics*, Vol. 57, No. 2, 1985, pp. 251-284.

56. Shih, T. M., Tan, C. H., and Hwang, B. C., "Effects of Grid Staggering on Numerical Schemes," *International Journal for Numerical Methods in Fluids*, Vol. 9, 1989, pp. 193-212.

57. Davis, R. T., "Laminar Incompressible Flow Past a Semi-Infinite Flat Plate," *Journal of Fluid Mechanics*, Vol. 27, No. 4, 1967, pp. 691-704.

58. Van De Vooren, A. I., and Dijkstra, D., "The Navier-Stokes Solution for Laminar Flow Past a Semi-Infinite Flat Plate," *Journal of Engineering Mathematics*, Vol. 4, No. 1, 1970, pp. 9-27.

59. Yoshizawa, A., "Laminar Viscous Flow Past a Semi-Infinite Flat Plate," *Journal of the Physical Society of Japan*, Vol. 28, No. 3, 1970, pp. 776-779.

60. Dennis, S. C. R., and Walsh, J. D., "Numerical Solutions for Steady Symmetric Viscous Flow Past a Parabolic Cylinder in a Uniform Stream," *Journal of Fluid Mechanics*, Vol. 50, No. 4, 1971, pp. 801-814.

61. Botta, E. F. F., Dijkstra, D., and Veldman, A. E. P., "The Numerical Solution of the Navier-Stokes Equations for Laminar, Incompressible Flow Past a Parabolic Cylinder," *Journal of Engineering Mathematics*, Vol. 6, No. 1, 1972, pp. 63-81.

62. Davis, R. T., "Numerical Solution of the Navier-Stokes Equations for Symmetric Laminar Incompressible Flow Past a Parabola," *Journal of Fluid Mechanics*, Vol. 51, No. 3, 1972, pp. 417-433.

63. Ghia, U., Ghia, K. N., and Shin, C. T., "High-Re Solutions for Incompressible Flow Using the Navier-Stokes Equations and a Multigrid Method," *Journal of Computational Physics*, Vol. 48, No. 3, 1982, pp. 387-411.

64. Schreiber, F., and Keller, H. B., "Driven Cavity Flows by Efficient Numerical Techniques," *Journal of Computational Physics*, Vol. 49, No. 2, 1983, pp. 310-333.

65. Nishida, H., and Satofuka, N., "Higher-Order Solutions of Square Driven Cavity Flow Using a Variable-Order Multi-Grid Method," *International Journal for Numerical Methods in Engineering*, Vol. 34, No. 2, 1992, pp. 637-653.

66. Guerrero, J. S. P., and Cotta, R. M., "Integral Transform Solution for the Lid-Driven Cavity Flow Problem in Streamfunction-Only Formulation," *International Journal for Numerical Methods in Fluids*, Vol. 15, No. 4, 1992, pp. 399-409.

67. Hansen, E. B., and Kelmanson, M. A., "An Integral Equation Justification of the Boundary Conditions of the Drive-Cavity Problem," *Computers and Fluids*, Vol. 23, No. 1, 1994, pp. 225-240.

68. Srinivasan, R., "Accurate Solutions for Steady Plane Flow in the Driven Cavity. I. Stokes Flow," *Zeitschrift fur Angewandte Mathematik und Physik*, Vol. 46, No. 4, 1995, pp. 524-545.

69. Gervais, J. J., Lemelin, D., and Pierre, R., "Some Experiments with Stability Analysis of Discrete Incompressible Flow in the Lid-Driven Cavity," *International Journal for Numerical Methods in Fluids*, Vol. 24, No. 5, 1997, pp. 477-492.

70. Barragy, E., and Carey, G. F., "Stream Function-Vorticity Driven Cavity Solution Using p Finite Elements," *Computers and Fluids*, Vol. 26, No. 5, 1997, pp. 453-468.

71. de Vahl Davis, G., "Natural Convection of Air in a Square Cavity: a Benchmark Numerical Solution," *International Journal for Numerical Methods in Fluids*, Vol. 3, 1983, pp. 249-264.

72. Hortmann, M., and Peric, M., "Finite Volume Multigrid Prediction of Laminar Natural Convection: Bench-Mark Solutions," *International Journal for Numerical Methods in Fluids*, Vol. 11, 1990, pp. 189-207.

73. Karniadakis, G. E., and Triantafyllou, G. S., "Three-Dimensional Dynamics and Transition to Turbulence in the Wake of Bluff Objects," *Journal of Fluid Dynamics*, Vol. 238, 1992, pp. 1-30.

74. Mittal, R., and Balachandar, S., "Effect of Three-Dimensionality on the Lift and Drag of Nominally Two-Dimensional Cylinders," *Physics of Fluids*, Vol. 7, No. 8, 1995, pp. 1841-1865.

75. Barkley, D., and Henderson, R. D., "Three-Dimensional Floquet Stability Analysis of the Wake of a Circular Cylinder," *Journal of Fluid Dynamics*, Vol. 322, 1996, pp. 215-241.

76. Balachandar, S., Mittal, R., and Najjar, F. M., "Properties of the Mean Recirculation Region in the Wakes of Two-Dimensional Bluff Bodies," *Journal of Fluid Dynamics*, Vol. 351, 1997, pp. 167-199.

77. Gartling, D. K., "A Test Problem for Outflow Boundary Conditions-Flow Over a Backward-Facing Step," *International Journal for Numerical Methods in Fluids*, Vol. 11, 1990, pp. 953-967.

78. Gresho, P. M., Gartling, D. K., Torczynski, J. R., Cliffe, K. A., Winters, K. H., Garratt, J. T., Spence, A., and Goodrich, J. W., "Is the Steady Viscous Incompressible Two-Dimensional Flow Over a Backward-Facing Step at Re=800 Stable?," *International Journal for Numerical Methods in Fluids*, Vol. 17, 1993, pp. 501-541.

79. Guerrero, J. S. P., and Cotta, R. M., "Benchmark Integral Transform Results for Flow Over a Backward-Facing Step," *Computers and Fluids*, Vol. 25, No. 5, 1996, pp. 527-540.

80. Blackwell, B. F., and Pepper, D. W., eds. *Benchmark Problems for Heat Transfer Codes*,

Vol. ASME HTD-Vol. 222, 1992, American Society of Mechanical Engineers, New York, NY.

81. Blackwell, B. F., and Armaly, B. F., eds. *Computational Aspects of Heat Transfer: Benchmark Problems*, Vol. ASME HTD-258, 1993, American Society of Mechanical Engineers, New York, NY.

82. Lin, S. J., Barson, S. L., and Sindir, M. M., "Development of Evaluation Criteria and a Procedure for Assessing Predictive Capability and Code Performance," 1992, pp. 11.

83. Marvin, J. G., "Perspective on Computational Fluid Dynamics Validation," *AIAA Journal*, Vol. 33, No. 10, 1995, pp. 1778-1787.

84. Cosner, R. R., "CFD Validation Requirements for Technology Transition," AIAA Paper No. 95-2227, *26th AIAA Fluid Dynamics Conf.*, San Diego, CA, 1995.

85. Sindir, M. M., Barson, S. L., Chan, D. C., and Lin, W. H., "On the Development and Demonstation of a Code Validation Process for Industrial Applications," AIAA Paper No. 96-2032, *27th AIAA Fluid Dynamics Conf.*, New Orleans, LA, 1996.

86. Sindir, M. M., and Lynch, E. D., "Overview of the State-of-Practice of Computational Fluid Dynamics in Advanced Propulsion System Design," AIAA Paper No. 97-2124, 1997.

87. ISO, "Guide to the Experssion of Uncertainty in Measurement," International Standards Organization, ISBN 92-67-10188-9, Geneva, Switzerland

88. AIAA, "Assessment of Wind Tunnel Data Uncertainty," American Institute of Aeronautics and Astronautics, S-071-1995, Washington, DC

89. Oberkampf, W. L., and Aeschliman, D. P., "Joint Computational/Experimental Aerodynamics Research on a Hypersonic Vehicle: Part 1, Experimental Results," *AIAA Journal*, Vol. 30, No. 8, 1992, pp. 2000-2009.

90. Walker, M. A., and Oberkampf, W. L., "Joint Computational/Experimental Aerodynamics Research on a Hypersonic Vehicle: Part 2, Computational Results," *AIAA Journal*, Vol. 30, No. 8, 1992, pp. 2010-2016.

91. Aeschliman, D. P., and Oberkampf, W. L., "Experimental Methodology for Computational Fluid Dynamics Code Validation," Sandia National Labs., SAND95-1189, Albuquerque, NM, Sept. 1997.

92. Oberkampf, W. L., Aeschliman, D. P., Henfling, J. F., and Larson, D. E., "Surface Pressure Measurements for CFD Code Validation in Hypersonic Flow," AIAA Paper No. 95-2273, *26th Fluid Dynamics Conf.*, San Diego, CA, 1995.

93. Desideri, J. A., Glowinski, R., and Periaux, J., eds. *Hypersonic Flows for Reentry Problems*, 1991, Springer-Verlag, Berlin.

94. Settles, G. S., and Dodson, L. J., "Hypersonic Shock/Boundary-Layer Interaction Database," NASA, Contractor Rept. 177577, April 1991.

95. Holden, M. S., and Moselle, J. R., "A Database of Aerothermal Measurements in Hypersonic Flow for CFD Validation," AIAA Paper No. 92-4023, *AIAA 17th Aerospace Ground Testing Conf.*, Nashville, TN, American Institute of Aeronautics and Astronautics, 1992.

96. Settles, G. S., and Dodson, L. J., "Hypersonic Turbulent Boundary-Layer and Free Shear Layer Database," NASA, Contractor Rept. 177610, April 1993.

97. Bertin, J. J., Martellucci, A., Neumann, R. D., and Stetson, K. F., "Developing a Data Base for the Calibration and Validation of Hypersonic CFD Codes - Sharp Cones," AIAA Paper No. 93-3044, *24th AIAA Fluid Dynamics Conf.*, Orlando, FL, 1993.

98. Holden, M. S., Moselle, J. R., Sweet, S. J., and Martin, S. C., "A Database of Aerothermal Measurements in Hypersonic Flow for CFD Validation," AIAA Paper No. 96-4597, *AIAA 7th International Space Planes and Hypersonic Systems and Technologies Conf.*, Norfolk, VA, 1996.